THERMODYNAMIC CONDITIONS OF ta-C FORMATION AT IMPLANTATION OF NOBLE-GAS IONS IN CARBON

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Abstract

Tetrahedral amorphous carbon (ta-C) formation at implantation of noble gas ions with energy from 25 to 1000 eV in carbon target is investigated in the model of thermoelastic peak (TEP). The dependences of radius, temperature and pressure in TEP on the ion energy were obtained. The *P,T* - trajectories of the points corresponding to the matter state in ion TEPs during acoustic and thermal relaxation were set on the phase *P,T*- diagram of carbon. The possibility of ta-C formation in TEP was qualitatively investigated from location of trajectory relative to boundary line "diamond - graphite". The effectiveness of «$sp^2 \rightarrow sp^3$» rearrangements in TEP was determined depending on sort and energy of the ion.

INTRODUCTION

As is known, the treatment of carbon by low-energy ions can promote its transformation to tetrahedral amorphous carbon (ta-C) [1]. There was intensive investigation of ta-C formation at $^{12}C^+$ ion implantation in carbon target (see, e.g. [1] and references there). The thermodynamic conditions of ta-c formation at implantation of C^+ ion in carbon were investigated theoretically in [2]. By hypothesis, these conditions are realized due to high temperature and pressure in thermoelastic peaks (TEPs) – nanometer-scale regions of matter where thermalized energy and volume of implanted ion are localized. The main features of this approach are taking into account the finiteness of initial dimension and origin time of TEP, as well as a combined action of temperature and all components of pressure in TEP on the rearrangement process.

In this paper, in the framework of the TEP concept [2], we perform a comparative analysis of conditions of ta-C formation at implantation of Ne^+ Ar^+, Kr^+ and Xe^+ ions with energy from 25 eV to 1000 eV in carbon. The effectiveness of ta-C formation in TEPs of noble gas ions was calculated.

RESULTS AND CONCLUSIONS

According to results of TRIM simulation, one can approximate TEPs of considered ions by spherical regions containing from 40 to 2000 atoms. It justifies correctness of the suggested thermodynamic approach. The radius, energy and lifetime of TEPs caused by noble gas ions were determined on the basis of TRIM simulation of ion-to-matter energy transfer and taking into account relaxation processes. Temperature in TEP was determined from phonon component of ion energy loss in TEP's volume. Thermoelastic, deformation and residual components of pressure in TEP have been found using radiation acoustic equations. Calculation has shown that temperature and all components of pressure in TEPs depend considerably on sort and energy of the ion.

The initial positions and trajectories of points corresponding to TEPs matter state on *P,T* phase diagram of carbon were determined (see Figure 1). Here dash-dot lines separate stability regions of different phases whereas dotted lines show initial locations of TEPs of specific ions. The sharp pressure decay on initial stage of the peak evolution corresponds to the acoustic wave escape almost without cooling. After that, pressure achieves the quasi-static level and decreases in accordance with increase of TEP volume. Analysis shows that trajectories of TEPs generated by ions with energy $E<E_1$ ($E>E_2$) lie entirely in the region of diamond (graphite) stability. Hence, ions with energies $E<E_1$ produce high concentration of ta-C whereas the ones with $E>E_2$ do not produce ta-C at all. Here $E_1 \approx 75$, 150, 150, 200 eV and $E_2 \approx 450$, 900, 750, 600 eV for ions Ne^+, Ar^+, Kr^+, Xe^+, correspondingly. The ions with energies $E_1 < E < E_2$ also produce ta-C but its concentration decreases with increase of the ion energy.

The total number W(E) of sp^2 to sp^3 transitions in ion TEP under combined action of temperature and pressure was used as a factor of effectiveness of ta-C formation. As one can see from Figure 2 the effectiveness of ta-C formation

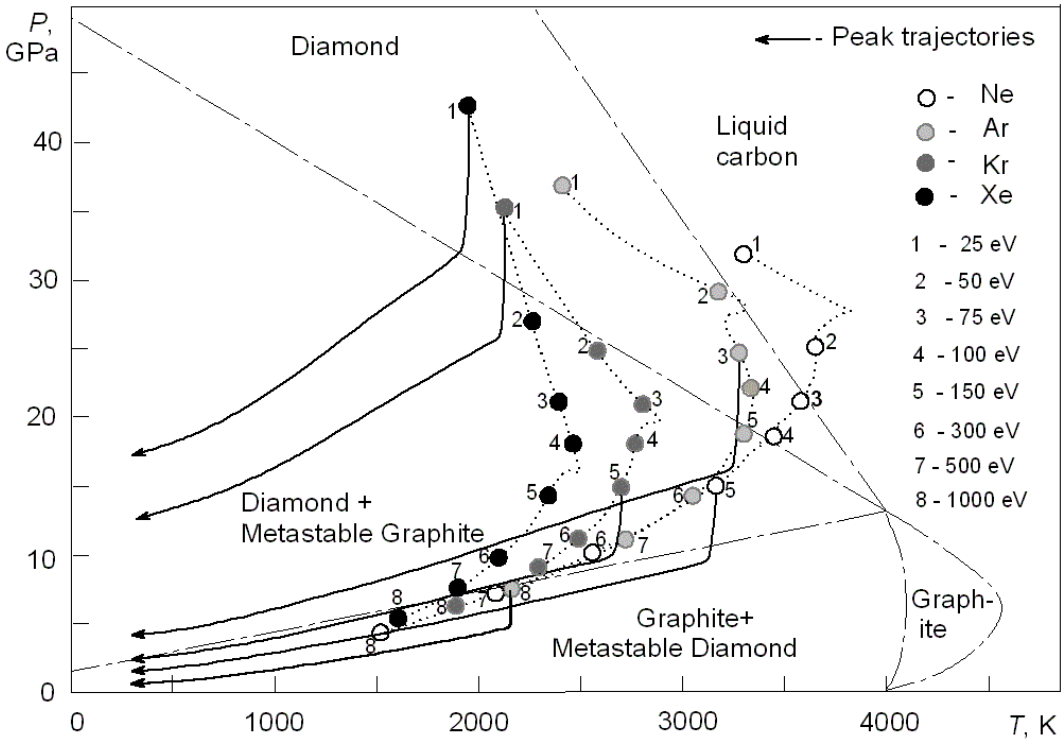

Figure 1. Location of P,T-trajectories (solid lines) of TEPs of noble gas ions on phase diagram of carbon.

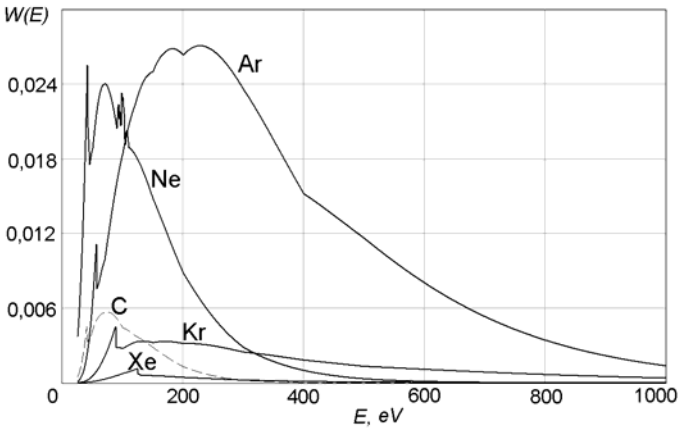

Figure 2. Energetic dependence of number of rearrangements $sp^2 \rightarrow sp^3$ in TEPs of C^+ and noble gas ions in carbon.

depends considerably on the ion sort. The maximal effectiveness is observed for Ar^+ and Ne^+, the minimal one is for Xe^+. The maxima of effectiveness for different ions are observed at different energies. Moreover, there are several peaks on the curves of effectiveness of ta-C formation for different ions: at 40, 60 and 90 eV for Ne^+ , at 56 and 200 eV for Ar^+, at 90 and 150 eV for Kr^+. The presence of two peaks in sp^3 content of carbon target after Ar^+ ion treatment is experimentally justified [3]. The dense phase formation in TEPs of Ar^+ and Kr^+ ions with energy ≤1000 eV occurs with an appreciable rate whereas the rates of the structural rearrangement to sp^3 state in TEPs of C^+, Ne^+ and Xe^+ of such energies are negligible.

REFERENCES

1. Hofsäss, H., et al. "Cylindrical spike model for the formation of diamondlike thin films by ion deposition," *Appl. Phys. A: Materials Science and Processing*, Vol. 8, pp.1351-1363 (1998).
2. Kalinichenko A.I., Strelnytskiy V.E. "Role of thermoelastic stress in formation of diamond-like coating at irradiation of amorphous carbon by low-energy C^+ ions," *Physics and Chemistry of Material Processing*, No 2, pp. 5-10 (2003). (In Russian.)
3. Patsalas P., et al. "Surface-activation processes and ion-solid interactions during the nucleation and growth of ultra-thin amorphous carbon films," *Thin Solid Films*, Vol. 428 pp.211-215 (2003).